ABSTRACT

It is an object of the present invention to provide a method of efficiently and rapidly determining the assignment of signals obtained by the ^{1}H-^{15}N HSQC measurement or the like, and a method of efficiently and rapidly identifying the three-dimensional structure of a target protein using the above method or a method of identifying the binding site of a protein of interest to a ligand, in place of the conventional signal assignment method, which requires a protein with a concentration several to 10 times higher than the lowest concentration of a protein capable of being observed by a high sensitive ^{1}H-^{15}N HSQC measurement method. In the present invention, ^{15}N/^{13}C double-labeled amino acids, ^{15}N-labeled amino acids, and non-labeled amino acids are systematically combined and used as substrates with respect to every amino acids constituting a protein of interest, so as to synthesize multiple proteins (20 types or 39 types of proteins at the maximum), and the NMR measurement is performed on such multiple proteins by a measurement method capable of identifying the correlation signals of two amino acid residues adjacent to each other, and then the obtained signals are compared.